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LANSCE DIVISION RESEARCH REVIEW

Designing Neutron Scattering and Optics Instruments with a Versatile Monte Carlo Tool Developed at LANSCE

L. L. Daemen, P. A. Seeger, R. P. Hjelm, and T. G. Thelliez (LANSCE-12)

Neutron-scattering experiments require carefully designed instruments that will ensure optimal use of the beam. Unlike x-rays, neutron sources have inherently low brightness and neutrons are very expensive to produce. Designing and building an instrument to "match" the neutron source is more cost effective than modifying the source itself. The ideal scheme would be to optimize the performance of a neutron-scattering instrument and its optics to match the moderator characteristics during the instrument's design phase. We have done just that, drawing upon the experience of pioneers in the computer simulation of neutron-scattering problems, including Johnson and Stephanou,[1,2] who developed the original concept of a library of Monte Carlo subroutines for neutron optics. We have developed a public-access software program, the Neutron Instrument Simulation Package (NISP), which provides instrument designers with a general, versatile Monte Carlo tool that simulates neutron-scattering instruments while taking into account the imperfections associated with optical components.

"Cradle to Grave" Simulation Capability

NISP is a versatile and general computer simulation package that allows users to design and test a wide range of neutron scattering instruments or to simulate an experiment using computer models of instruments already created (and archived) with NISP. Users can track the history of a neutron as it journeys from the moderator to the detector. Neutron-optic models describe neutron transport and scattering as neutrons interact with the optical elements and other components on their simulated journey through an instrument. Users can monitor intermediate results such as neutron detection events in a detector, or they can visualize an instrument as a three-dimensional (3D) model (Fig. 1); manipulate a component by simply clicking on its picture; verify instrument geometry while constructing the model; and zoom in and out, change scale, rotate, translate, etc., with this unique program. NISP runs on UNIX, Linux, Windows, Mac, and DEC platforms.

The three main programs that comprise NISP are MCLIB, MC_RUN, and MC_Web. MCLIB is a library of Fortran subroutines that handles geometry representations, neutron-transport algorithms, and optical-element models. MC_RUN is a Monte Carlo engine that runs a simulation and produces a series of output files with detector counts and general information about the progress and outcome of the simulation. MC_Web is a user-friendly Web-based application that allows the designer to set up the instrument geometry interactively without having to learn the MCLIB data structures. NISP has a tutorial to help users build their instruments or run experiments on existing models. By registering online at http://strider.lansce.lanl.gov/NISP/Welcome.html,

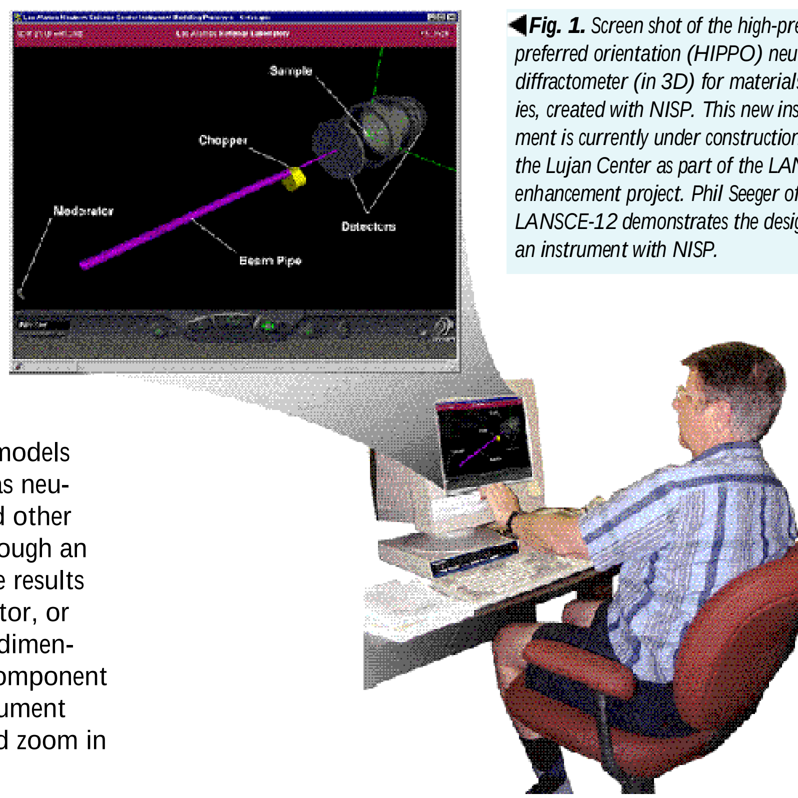


Fig. 1. *Screen shot of the high-pressure preferred orientation (HIPPO) neutron diffractometer (in 3D) for materials studies, created with NISP. This new instrument is currently under construction at the Lujan Center as part of the LANSCE enhancement project. Phil Seeger of LANSCE-12 demonstrates the design of an instrument with NISP.*

users will be kept informed of new features and revisions to the code via the "What's New" link on the MC_Web login page. A tutorial, a manual, and documentation are also available online. And users can download source code and executables free at http://strider.lansce.lanl.gov/NISP/Welcome.html to their computers to produce computer models of an instrument and run simulations to test its performance quantitatively, or they can run simulations of experiments on instrument models already created with NISP.

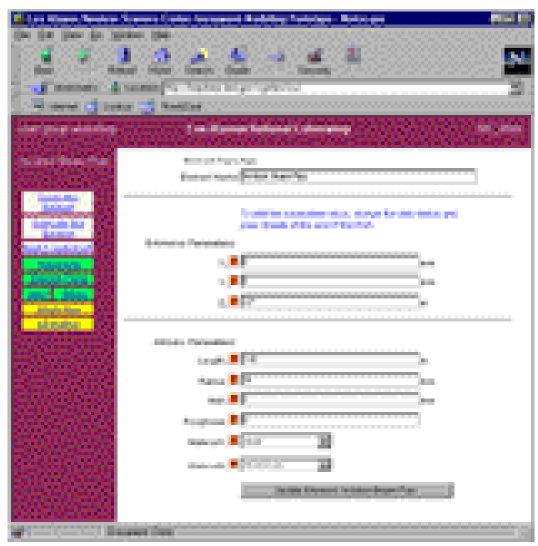
Instrument Simulation—Then and Now

The pulse emitted by a moderator at a pulsed neutron source has a complicated dependence on time, energy, and direction of emission. Because these factors impact the performance of an instrument, they must be taken into account during the design of the instrument. Moreover, many imperfections in the optical elements of an instrument can influence the instrument's performance—these effects, however, cannot be anticipated nor calculated very easily. In 1993, we began looking at the development of a tool that was needed to design an instrument suite for the LANSCE-II project. By 1994, we restructured and expanded the MCLIB code by Johnson,[1,2] and generalized existing single-purpose instrument-simulation codes to create MC_RUN.

Work began in earnest on a user interface[3] for NISP in 1995, and in 1996 the first prototype was successfully tested in time for the start of the LANSCE Enhancement Project. By 1997, we had published many applications and created a Web interface called MC_Web to allow users free access to source code and executables. In November 1997, a committee was formed to oversee the creation of an international standard for Monte Carlo libraries for instrument simulation and to develop a methodology for code maintenance and distribution. Since 1998, we have added to MCLIB a Fermi chopper, curved crystal, curved neutron guide, multi-level inelastic scattering sample, and a more general crystal model where the lattice planes are not necessarily parallel to the crystal. New elements continue to be added, and more sophisticated algorithms are being introduced for existing elements (Figs. 2 and 3). In 1999, we began working on neutron polarization and the addition of components that act on neutron spin. This new feature is important for the construction of neutron-scattering instruments geared toward the study of magnetism in matter.

This unique Monte Carlo tool automatically deals with unexpected events and takes into account the

▲ ***Fig. 2.*** *Screen shot of a list of elements that can be accessed through MCWeb and incorporated in the design of an instrument. Each optical element is "pre-packaged" with an associated geometry and properties as defined in MCLIB.*



▲ ***Fig. 3.*** *Screen shot of the form used to define an element to be incorporated in an instrument. Users can add their own element types or use a large library of pre-defined elements. An online help feature assists users in defining each element and parameter.*

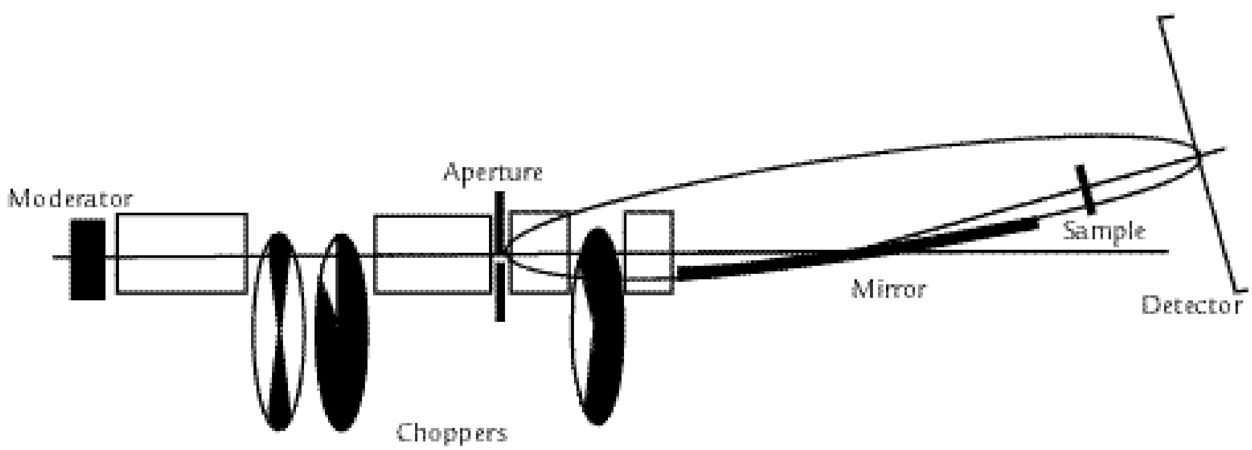
imperfections of instrument elements, such as surface roughness and chopper jitter, and complex element features, such as the time-energy distribution of the neutron pulse. The program allows users to integrate simulations over a large number of instrument parameters and gain access to detailed information that is otherwise not easily obtainable experimentally, like true neutron energy in time-of-flight methods. Idealized samples help calculate hard-to-obtain instrument characteristics, and realistic data sets provided by the program allow users to try a variety of analysis techniques. Elements or element features can be turned on and off, or can be adjusted continuously, thereby allowing the user to assess their impact on instrument performance, which is not usually possible in an actual experiment. For instance, the mosaic spread of a crystal monochromator can be set to any statistical distribution or ignored altogether—an impossible feat to accomplish with a real crystal.

Comparing Mirror Efficiency with NISP

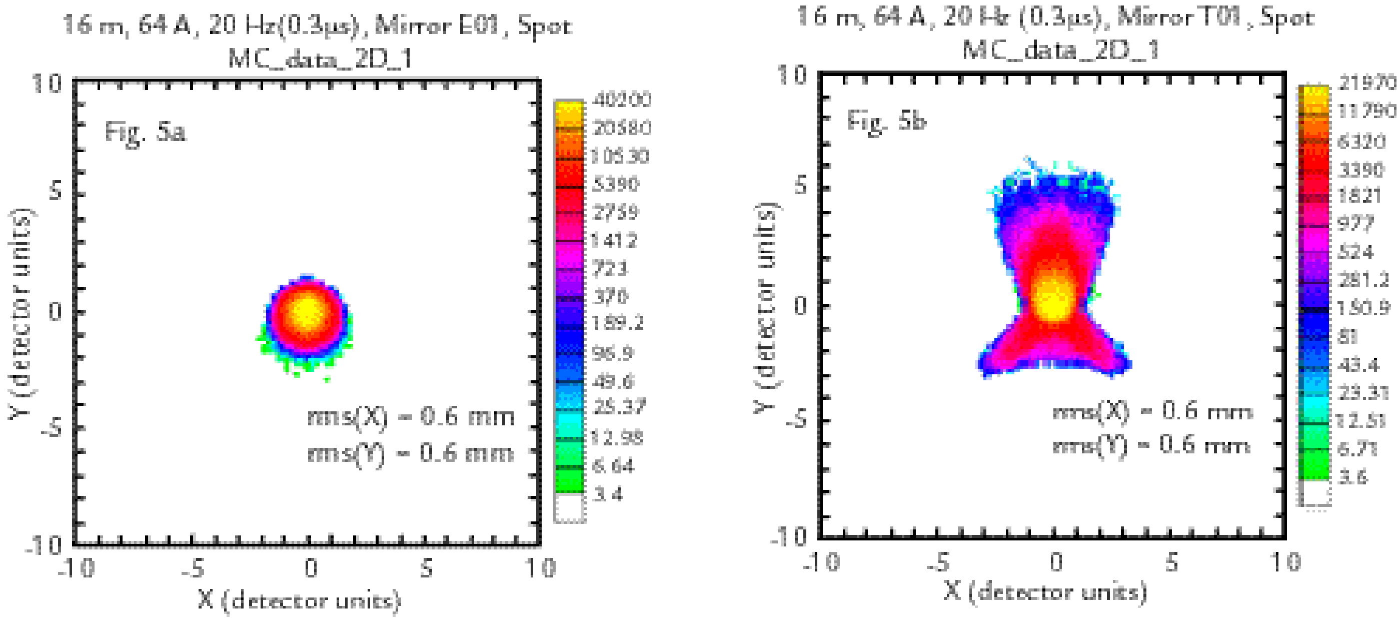
Figure 4 represents the configuration of a small-angle neutron-scattering instrument in the design phase, shown here as an example of the type of studies that have been performed using NISP. A mirror with the shape of a portion of an ellipsoid was incorporated into the NISP design. A useful feature of the ellipsoidal shape is that rays (in this case, neutrons) passing through one focus are reflected to pass through the other focus. We thus form an image of the collimating aperture (placed at the first focus) at the surface of the detector (placed at the second focus). When a sample is placed in the beam, neutrons are scattered at various angles, revealing long-range structure in the sample. Since the resolution of the scattering angle depends on the size of the beam spot, focusing increases count rate without spoiling resolution. MCLIB deals with all the physical interactions felt by the neutron from its emission by the moderator to its detection in the detector—transmission through the choppers, aperture, and drift spaces; reflection on the mirror surface; and small-angle scattering in the sample.

Toroidal mirrors are sometimes used to approximate an ellipsoid because they are less expensive and easier to fabricate. We used NISP to simulate an instrument with an ellipsoidal mirror so that we could compare the instrument performance with a toroidal mirror and with an ellipsoidal mirror. The results of two NISP simulations are shown in Fig. 5. The ellipsoidal mirror (Fig. 5a) behaves well—the largest apparent defocusing effect is gravity. The toroidal mirror (Fig. 5b) produces a grossly distorted image of the source. Notice that in both cases, the yellow spot at the center of the image is the answer that a simple ray-tracing approach of first-order geometric optics (ignoring aberrations) would have given.

In developing NISP, we have tried to be responsive to the needs of the neutron-scattering community. Our work can go forward only with input and feedback from the user community. We encourage users to send comments, criticisms, and requests for additional features. Much code has been written over the years to simulate very specific optical elements and neutron-scattering processes. In a number of cases, we have incorporated this legacy code in NISP to mutually benefit the author and other users of the code.



▲ ***Fig. 4.*** *A typical small-angle neutron-scattering instrument with an ellipsoidal mirror, which is used to increase neutron flux on sample. A neutron emitted by the moderator travels down the instrument axis, through the aperture, and hits the ellipsoidal mirror. The neutron is reflected, then scattered by the sample, and detected in the position-sensitive detector. The spatial distribution of neutron intensity in the detector reflects certain features of the microstructure of the sample material.*



▲ ***Fig. 5.*** *A comparison between the image of a 2-mm-diam aperture produced by an ellipsoidal mirror (a) and a toroidal mirror (b).*

References

1. M.W. Johnson and C. Stephanou, "MCLIB: A Library of Monte Carlo Subroutines for Neutron Scattering Problems," Rutherford Appleton Laboratory report RL-78-090 (1978).

2. M.W. Johnson, "MCGUIDE: A Thermal Neutron Guide Simulation Program," Rutherford Appleton Laboratory report RL-80-065 (1980).

3. T.G. Thelliez, L.L. Daemen, P.A. Seeger, and R.P. Hjelm, "A User-Friendly, Graphical Interface for the Monte Carlo Neutron Optics Code MCLIB," in *Proceedings of the Thirteenth Meeting of the International Collaboration on Advanced Neutron Sources* **1**, 307-311 (1995).

For more information, contact Luke Daemen (LANSCE-12),505-667-9695, MS H805, lld@lanl.gov.

Produced by the LANSCE communications team: Barbara Maes, Sue Harper, Garth Tietjen, AnnMarie Dyson, and Grace Hollen.

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